New Type of Crystalline "Defect" Discovered

"Chevron" Structure Found at Metal Grain Boundaries

Using atomic resolution electron microscopy, scientists at LBNL's National Center for Electron Microscopy (NCEM) have discovered a new type of crystalline "defect" that forms at boundaries between grains in polycrystalline metals. The defect occurs at the line of intersection between certain grain boundaries and surfaces and takes the form of a chevron-like, V-shaped region less than 5 nm across. This discovery has implications for grain growth in polycrystalline materials, the equilibrium structure of grain boundaries, and the possibility of stabilizing new phases in the nanoscale size regime.

Structures formed at grain boundaries are of fundamental importance in determining the physical properties of polycrystalline materials. Nearly all structural metals are used in their polycrystalline form and the structure and composition of their grain boundaries affects their superplastic deformation, embrittlement, corrosion, and electronic or superconducting behavior.

The local atomic structure of a material is altered at grain boundaries to accommodate the deviation from the crystalline order of the bulk material. The structure in these regions depends on a combination of a number of macroscopic crystallographic parameters and on the atomic interactions characteristic for the material. Great progress has been made in recent years in our understanding of grain boundary behavior by correlating experimental observations with atomistic simulations. A particularly notable advance was the discovery of "grain boundary dissociation" in materials such as copper, with low "stacking fault" energy, the increase in energy due to a mistake in the stacking sequence of densely packed crystal planes. In this phenomenon, rather than forming immediately adjacent to one another, two grains are separated by a solid wetting layer of the same composition as the adjoining grains, but differing in structure or orientation.

In research reported here, NCEM's new One-Ångstrom Microscope was employed to examine regions in gold where the grain boundary reaches a free surface. It was found that, in this area, a small chevron-shaped "defect" region is formed that has a different crystalline structure from either of the adjacent grains (see figure). This region can be considered the one-dimensional equivalent of the solid wetting layer described above as grain boundary dissociation. Detailed examination clearly reveals that it is formed from a series of "stacking faults" parallel to the two inclined sides. Atomistic simulations confirmed that the observed structure corresponds to an energy minimum and predicted that the structure should be stable only over a narrow size range of a few nanometers, in agreement with observation.

Defects of this type had not been reported previously. Although the new phenomenon has been, to date, observed only in gold, it is expected to occur more generally in all materials with low stacking fault energy. The defects may also be considered a dissociation of a line junction between a grain boundary and a surface, or the wetting of such a line by a solid "wire" of different structure. This solid "wire" is naturally limited to nanometer dimensions in the direction normal to the junction line. By exploiting the principles first demonstrated in this work, it may eventually become possible to generate nanowires of specific sizes and shapes and to control their position and orientation.

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T. Radetic, F. Lançon, and U. Dahmen, "Chevron Defect at the Intersection of Grain Boundaries with Free Surfaces in Au," *Phys. Rev. Lett*. **89**, 085502 (2002).